Interstitial Order-Disorder Transformation in the Ti-O Solid Solution: III. A Statistical Theory

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<th>語学での論文表示記載の詳細</th>
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<tbody>
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<td>論文の詳細は上記のURLを参照</td>
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Interstitial Order–Disorder Transformation in the Ti–O Solid Solution. III. A Statistical Theory*

Masahiro KOIWA and Makoto HIRABAYASHI

The Research Institute for Iron, Steel and Other Metals

Abstract

A theory of the interstitial order–disorder transformation in the h.c.p. lattice has been developed on the basis of the Bragg-Williams approximation. The calculated results are compared with the experiments on the Ti–O system reported in Part I and Part II. Oxygen atoms situated on the octahedral interstices are considered to repel each other. As the interstitial disordering proceeds in the two successive steps of the intra- and inter-plane disordering, analytical calculations are made by treating the two processes independently. Then numerical computations are carried out taking account of mutual correlations of these processes. It is revealed that the intra-plane disordering is considerably modified by simultaneous occurrence of the inter-plane disordering. The transformation energy and entropy are deduced as a function of oxygen contents. A tentative phase diagram is constructed by evaluating the repulsive energies for three pairs of the oxygen atoms. These results are consistent with the characteristic features observed experimentally, but some discrepancies are noted on the inter-plane disordering.